

Sulfone, methyl pentafluorophenyl  
651-85-4 | DTXSID30215403

Model Performance

Model	Data
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Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.85	0.69	0.86	0.67	0.86	0.78

Model Results

Predicted value: 4.81

Global applicability domain: Inside

Local applicability domain index: 3.63e-01

Confidence level: 6.64e-01

Nearest Neighbors from the Training Set

Image not found  
Tricyclo[8.2.2.24,7]hexadeca-  
4,6,10,12,13,15-hexaene  
**Measured:** 4.33  
**Predicted:** 5.02

Image not found  
Dihydropyrene  
**Measured:** 4.92  
**Predicted:** 3.05

Image not found  
1,1'-(2,2-Dichlorocyclopropane-  
1,1-diyl)dibenzene  
**Measured:** 4.88  
**Predicted:** 5.75

Image not found  
9,10-Dimethylantracene  
**Measured:** 5.69  
**Predicted:** 3.36

Image not found  
Anthracene, 9,10-dihydro-  
**Measured:** 4.25  
**Predicted:** 2.96